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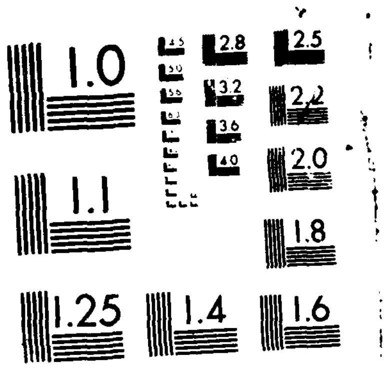
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Center for Multivariate Analysis
University of Pittsburgh

December 1986

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Center for Multivariate Analysis
Fifth Floor Thackeray Hall
University of Pittsburgh
Pittsburgh, PA 15260

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In this paper, the authors studied certain properties of the estimate of Liang and Krishnaiah (*J. Multivariate Anal.*, 16, 162-172) for multivariate binary density. An alternative shrinkage estimate is also obtained. The above results are generalized to general orthonormal systems.

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1. INTRODUCTION

In a number of situations, the experimenter is confronted with the statistical analysis of the data which is binary in nature. For example, one may be interested in diagnosis of the disease on the basis of symptoms. The reliability of complicated systems can be studied by examining as to whether its components are functioning or not. In image processing, a picture is classified on the basis of two gray levels like white and black using some threshold value. We may assign a score of 1 or 0 according as the grey level is white or black respectively. So, it is important to study the problems of estimation of multivariate binary density.

Cencov [3] expressed continuous multivariate density as a series of orthonormal functions. Bahadur [1] expressed the multivariate binary density as a series. Ott and Kronmal [5] expressed the density as a series involving Walsh functions. Liang and Krishnaiah [4] also expressed the density in terms of Walsh functions but the coefficients in their series are different from those used by Ott and Kronmal. Th ~~The present~~ paper is a continuation of the work done by Liang and Krishnaiah.

In Section 2, we established the necessary and sufficient condition for the difference between the mean integrated square error (MISE) of the estimate of Liang and Krishnaiah and the MISE of a "natural" shrinkage estimator to be of order $O(n^{-2})$ where n denotes the sample size. It is also shown that $O(n^{-2})$ is the best possible rate that can be obtained. In Section 3, a new shrinkage estimate of the multivariate binary density estimate is proposed. It is shown that the difference between the MISE of this estimate and the "natural" shrinkage estimator is of order $O(n^{-2})$. The results of Sections 2 and 3 are generalized to general orthonormal systems in Section 4.

2. SHRINKAGE ESTIMATES BASED ON WALSH FUNCTIONS

Denote by R the sets

$$R = \{(x_1, \ldots, x_d). \quad X_1 = 0 \text{ or } 1, \quad i = 1, \ldots, d\} \tag{1}$$

and by $\tilde{P} = \{p(x)\}$ the family of probability functions on R : $\tilde{P}$ includes all such function on R satisfying

$$p(x) \geq 0 \quad \text{for} \quad x \in R; \quad \sum_{x \in R} p(x) = 1. \tag{2}$$

The system of Walsh functions $\{\emptyset_r\}$ is defined by

$$\emptyset_r(x) = (-1)^{r'x}/2^{d/2}, \quad x \in R : r \in R. \tag{3}$$

Each $p(x) \in \tilde{P}$ can be expressed as

$$p(x) = \sum_{r \in R} a_r \emptyset_r(X). \tag{4}$$

So the estimation of $p(x)$ involves that of $\{a_r\}$.

Suppose that X is a random vector with range R whose distribution $p(x)$ is unknown, and $X_1, \ldots, X_n$ are iid. observations of X. Then, since

$$a_r = E\emptyset_r(X), \quad r \in R, \tag{5}$$

we obtain the moment estimate of a_r as

$$\hat{a}_r = \sum_{i=1}^{n} \emptyset_r(X_i)/n. \tag{6}$$

As argued in [4], there are reasons to consider the "shrinkage estimator"

$$\hat{p}_\lambda(x) = \sum_{r \in R} \lambda_r \hat{a}_r \emptyset_r(x) \tag{7}$$

in replacing the "natural" estimator $\hat{p}(x) = \sum_{r \in R} \hat{a}_r \emptyset_r(x)$ derived directly from (4) and (6). As was shown in [4], the mean integrated square error

of $\hat{p}_\lambda(x)$ to be denoted by MISE $(\hat{p}_\lambda)$, attains its minimum upon choosing

$$\lambda_r = na_r^2/(2^{-d} + (n-1)a_r^2), \quad r \in R. \tag{8}$$

Since in practice we do not know $\{a_r\}$, the constants $\{\lambda_r\}$ need to be estimated from the sample. Liang and Krishnaiah proposed such an estimate in [4] via some iteration considerations, as follows.

$$\lambda_r^* \begin{cases} 0, & \text{if } \hat{a}_r^2 < 4(n-1)2^{-d}/n^2 \\ [n + (n^2 - 4(n-1)2^{-d}\hat{a}_r^{-2})^{1/2}]/2(n-1), & \text{otherwise.} \end{cases} \tag{9}$$

Denote

$$\hat{p}_{\lambda *}(x) = \sum_{r \in R} \lambda_r^* \hat{a}_r \emptyset_r(x). \tag{10}$$

Liang and Krishnaiah proved the following theorem.

THEOREM ([4], Theorem 2). If $0 < |a_r| < 2^{-d/2}$ for all r, then [1)]

$$\text{MISE}(\hat{p}_{\lambda *}) - \text{MISE}(\hat{p}_\lambda) = O(n^{-2}). \tag{11}$$

Here we improve and complete this result as follows:

THEOREM 1. 1°. The necessary and sufficient condition for (11) to be true is that

$$a_r \neq 0, \quad \text{for all } r \in R. \tag{12}$$

---

1) We point out here that "$0 < |a_r| < 2^{-d/2}$ for all r" should be corrected as "$0 < |a_r| < 2^{-d/2}$ for all $r \neq (0, 0, \ldots, 0)$", since $a_r = 2^{-d/2}$ for $r = (0, 0, \ldots, 0)$.

2°. $O(n^{-2})$ is the best rate obtainable. Suppose that a_r^* is any estimate of a_r (based on $X_1, \ldots, X_n$) and form the estimator $p^*(x) = \sum_{r \in R} a_r^* \emptyset_r(x)$. Then for at least one $p(x) \in \tilde{P}$, we have

$$\limsup_{n\to\infty} n^2 |\text{MISE}(p^*) - \text{MISE}(\hat{p}_\lambda)| > 0. \tag{13}$$

Proof. 1°. Since $\emptyset_r$ is bounded by 1 on R, and $\emptyset_r(X_1), \ldots, \emptyset_r(X_n)$ are iid. random variables with mean a_r, by Bennett inequality (see [2]), we have

$$P(|\hat{a}_r - a_r| \geq \varepsilon) \leq 2 \exp(- \frac{n\varepsilon^2}{2(1+\varepsilon)}) \tag{14}$$

for arbitrarily $\varepsilon > 0$. The validity of (14) does not depend on the value assumed by a_r. Use (14) to replace (4-5) of [4], and the rest of the proof for sufficiency runs exactly along the same way as in [4].

To prove the necessity of (12), suppose that $a_{r_0} = 0$ for some $r_0 \in R$. Denote by $\tilde{R}$ the set $\{r: r \in R;\ a_r \neq 0\}$. Then we have

$$|\text{MISE}(\hat{p}_\lambda^*) - \text{MISE}(\hat{p}_\lambda) - E(\lambda_{r_0}^* \hat{a}_{r_0})^2|$$

$$\leq \sum_{r \in \tilde{R}} |E(a_r - \lambda_r \hat{a}_r)^2 - E(a_r - \lambda_r^* \hat{a}_r)^2|. \tag{15}$$

In the proof of sufficiency, we actually proved that

$$|E(a_r - \lambda_r \hat{a}_r)^2 - E(a_r - \lambda_r^* \hat{a}_r)^2| = O(n^{-2}), \quad r \in \tilde{R}. \tag{16}$$

On the other hand, since $a_{r_0} = 0$, we have

$$\text{Var}(\hat{a}_{r_0}) = 2^{-d}/n.$$

Hence, by Central Limit Theorem, we obtain

$$\sqrt{n}\, \hat{a}_{r_0} \xrightarrow{L} N(0, 2^{-d}), \quad (n \to \infty). \tag{17}$$

From (9) we see that $\lambda_r^* \geq \frac{1}{2}$ when $\lambda_r^* \neq 0$. Therefore

$$\liminf_{n\to\infty} P(\lambda_{r_0}^* \geq \frac{1}{2}) \geq \liminf_{n\to\infty} P(\hat{a}_{r_0}^2 \geq 4(n-1)2^{-d}/n^2)$$

$$= 1 - \frac{1}{\sqrt{2\pi}} \int_{-2}^{2} e^{-t^2/2} dt \overset{\Delta}{=} g > 0. \tag{18}$$

So, when n is large, we have

$$P(\lambda_{r_0}^* \geq 1/2) \geq g/2. \tag{19}$$

Use again (17). We get for arbitrarily given $\varepsilon > 0$

$$\lim_{n\to\infty} P(|\hat{a}_{r_0}| \geq \varepsilon/\sqrt{n}) = 1 - \frac{1}{\sqrt{2\pi}} \int_{-\varepsilon 2^{d/2}}^{\varepsilon 2^{d/2}} e^{-t^2/2} dt \overset{\Delta}{=} h_\varepsilon. \tag{20}$$

Choose $\varepsilon > 0$ small enough. We have $h_\varepsilon > 1 - g/3$. Therefore, for n sufficiently large, we have

$$E(\lambda_{r_0}^* \hat{a}_{r_0})^2 \geq (\frac{1}{2} \frac{\varepsilon}{\sqrt{n}})^2 P(\lambda_{r_0}^* > \frac{1}{2}, \quad |\hat{a}_{r_0}| \geq \frac{\varepsilon}{\sqrt{n}})$$

$$\geq \varepsilon^2/4n(P(\lambda_{r_0}^* \geq \frac{1}{2}) + P(|\hat{a}_{r_0}| \geq \frac{\varepsilon}{\sqrt{n}}) - 1)$$

$$\geq \varepsilon^2/4n(g/2 + 1 - g/3 - 1) = g\varepsilon^2/24n. \tag{21}$$

From (15), (16) and (21), we see that (11) cannot be true.

2°. To prove the second part of this theorem, we proceed to show that, even in the case of $d = 1$, (13) holds.

In the case of $d = 1$, x can only take two values, 0 and 1, and we shall write $p(0) = p$, $p(1) = 1 - p(0) = q$. In this case, we have

$$a_0 = 1/\sqrt{2}, \quad a_1 = (2p - 1)/\sqrt{2}. \tag{22}$$

Suppose that (a_0^*, a_1^*) is an estimate of (a_0, a_1). Then, since it is well-known in the theory of point estimation that the estimate

$$\hat{a}_1 = \sqrt{2}\,\overline{X}_n - 1/\sqrt{2}$$

is admissible under quadratic loss $L(d, a_1) = (d - a_1)^2$. It follows that there exists $p \neq 0, 1$, such that

$$E_p(a_1^* - a_1)^2 \geq E(\hat{a}_1 - a_1)^2 = 2pq/n. \tag{23}$$

Here $\lambda_1 = (2p-1)^2/[(2p-1)^2 + 4pq/n]$, and simple manipulations shows that

$$E_p(\lambda_1\hat{a}_1 - a_1)^2 = (2p-1)^2 2pq/n + 0(n^{-2}). \tag{24}$$

Here $a_0 = 1/\sqrt{2}$, $\lambda_0 = 1$, $\emptyset_0(0) = \emptyset_0(1) = 1/\sqrt{2}$. Hence, $E_p(\lambda_0\hat{a}_0 - a_0)^2 = 0$. From this and (24), we see that, denoting $p^*(x) = \sum_{r=1}^{1} a_r'\emptyset_r(\lambda)$,

$$\text{MISE}_p(p^*) - \text{MISE}_p(\hat{p}_\lambda) \geq [1 - (2p-1)^2]2pq/n + 0(n^{-2}).$$

Since $p \neq 0, 1$, $[1 - (2p-1)^2]pq > 0$, and we have

$$\limsup_{n\to\infty} n^2|\text{MISE}_p(p^*) - \text{MISE}_p(\hat{p}_\lambda)| = \infty.$$

This proves (13).

The above method of proof can be extended to the general case of d without difficulty. We need only consider a subset of $\tilde{P}$ with the form

$$\tilde{P}_1 = \{p(x): p(x) \in \tilde{P},\ p(x^{(1)}) = p,\ p(x^{(2)}) = 1 - p,\ 0 < p < 1\}$$

where $X^{(1)}$, $X^{(2)}$ are two chosen points in R and $x^{(1)} \neq x^{(2)}$.

3. A NEW SHRINKAGE ESTIMATE

We see from Theorem 1 that in order to have (11), the condition (12) is necessary. In this section we shall introduce a new shrinkage estimator, for which (11) holds without any restriction on $\{a_r\}$. For this purpose, define

$$\hat{\lambda}_r = \begin{cases} n\hat{a}_r^2/(2^{-d} + (n-1)\hat{a}_r^2), & \text{if } |\hat{a}_r| \geq n^{-1/3} \\ 0 & , \text{ otherwise} \end{cases} \tag{25}$$

and the shrinkage estimator

$$\hat{p}_{\tilde{\lambda}}(x) = \textstyle\sum_{r\in R}\hat{\lambda}_r\hat{a}_r\phi_r(x). \tag{26}$$

THEOREM 2. For $\hat{p}_{\tilde{\lambda}}$ defined in (26), we have

$$\text{MISE}(\hat{p}_{\tilde{\lambda}}) - \text{MISE}(\hat{p}_{\lambda}) = O(n^{-2}). \tag{27}$$

Proof. The proof is a slight modification of the proof of Theorem 2 in [4]. First, according to (4-3) of [4], we need only to show that

$$E(a_r - \lambda_r'\hat{a}_r)^2 E(\lambda_r - \tilde{\lambda}_r)^2 = O(n^{-4}) \tag{28}$$

for each $r \in R$, where λ_i' lies between λ_r and $\tilde{\lambda}_r$. Consider separately two cases.

1°. $a_r = 0$. In this case, using Bennett inequality (14), we find that

$$P(\tilde{\lambda}_r \neq 0) = P(|\hat{a}_r| \geq n^{-1/3}) \leq 2\exp(-n^{1/3}/4) = O(n^{-4}).$$

Since $\tilde{\lambda}_r$ is bounded by 1, we get

$$E(\lambda_r - \tilde{\lambda}_r)^2 = E\tilde{\lambda}_r^2 = O(n^{-4}).$$

As a_r, λ_r', $\hat{a}_r$ are bounded, we get (28).

2°. $a_r \neq 0$. Again, using Bennett inequality, we have

$$P(|a_r - \hat{a}_r| \geq |a_r|/2) \leq e^{-cn}, \quad \text{for some } c > 0. \tag{29}$$

Put $f_n(t) = nt/(2^{-d} + (n-1)t)$. There exists $c_1 > 0$ such that $f_n'(t) \leq c_1 n^{-1}$ for $t \geq |a_r|^2/4$, and c_1 does not depend on n. Hence

$$|\lambda_r - \tilde{\lambda}_r| \leq c_1 n^{-1} |\hat{a}_r^2 - a_r^2|.$$

Since $E|\hat{a}_r^2 - a_r^2|^2 \leq 2E|\hat{a}_r - a_r|^2 = 2 \operatorname{Var}(\hat{a}_r) = 0(n^{-1})$, we have

$$E(\lambda_r - \tilde{\lambda}_r) = 0(n^{-3}). \tag{30}$$

On the other hand, we have

$$E(a_r - \lambda_r' \hat{a}_r)^2 \leq 2 \operatorname{Var}(\hat{a}_r) + E(1 - \lambda_r')^2. \tag{31}$$

We have

$$1 - \lambda_r = 0(n^{-1}) \tag{32}$$

and

$$1 - \tilde{\lambda}_r = 0(n^{-1}), \quad \text{when} \quad |\hat{a}_r| \geq |a_r|/2. \tag{33}$$

From (32)-(33), and observing that λ_r' lies between λ_r and $\tilde{\lambda}_r$, we get in view of (29)

$$\begin{aligned} E(1 - \lambda_r')^2 &\leq 0(n^{-2}) + P(|\hat{a}_r| < |a_r|/2 \\ &\leq 0(n^{-2}) + P(|\hat{a}_r - a_r| \geq |a_r|/2) \\ &= 0(n^{-2}). \end{aligned} \tag{34}$$

Since $\operatorname{Var}(\hat{a}_r) = 0(n^{-1})$, from (31) and (34) we get

$$E(a_r - \lambda_r'\hat{a}_r)^2 = O(n^{-1}). \tag{35}$$

From (30) and (35) we get (28), and the theorem is proved.

4. ESTIMATES BASED ON GENERAL ORTHONORMAL SYSTEM

In the above discussions we chose Walsh functions as our orthonormal system. There are infinitely many orthonormal systems which can be chosen for the estimation purpose. The particular choice depends upon convenience and the needs for applications. For instance, the following system

$$\phi_r(x_r) = 1, \quad \phi_r(x) = 0 \quad \text{for } x \neq x_r, \quad r \in R$$

leads to the usual frequency estimate and its shrinkage. We now indicate that the results of Sections 2 and 3 are still valid for any choice of orthonormal system $\{\phi_r\}$. The only modification is that in the definitions of λ_r, λ_r^* and $\tilde{\lambda}_r$ in (8), (9) and (25), 2^{-d} should be replaced by

$$b_r = \textstyle\sum_{r \in R} p(x)\phi_r^2(x). \tag{36}$$

THEOREM 3. Suppose that $\{\phi_r\}$ is any orthonormal function system on R, then the conclusions of Theorem 2 and Theorem 3 remain valid if the definitions of λ_r, λ_r^* and $\tilde{\lambda}_r$ are modified as stated earlier.

The proof is obvious, since in the proofs of Theorem 2 and Theorem 3, the special form of Walsh functions plays no special role, except one point which we now discuss.

In the proof of Theorem 1. 2°, we made use of the fact that $a_0 = 1/\sqrt{2}$ is a constant, so that $\lambda_0\hat{a}_0$ gives an exact estimation of a_0. In the general case this situation no longer holds. In general we have

$$\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} \phi_0(0) & \phi_1(0) \\ \phi_0(1) & \phi_1(1) \end{pmatrix}^{-1} \begin{pmatrix} p \\ 1-p \end{pmatrix}$$

or

$$a_0 = ap + b, \qquad a_1 = cp + d$$

for some known constants a, b, c, d. An inspection of the proof of Theorem 1, 2° convinces us that we have to prove that $(a\overline{X}_n + b,\ c\overline{X}_n + d)$ is an admissible estimate of (a_0, a_1) under quadratic loss. That is to say, if there exists an estimate (a_0^*, a_1^*) such that

$$E_p(a_0' - a_0)^2 + E_p(a_1' - a_1)^2 \leq (a^2 + c^2)p(1-p)/n \tag{37}$$

for all $p \in (0, 1)$, then in (37) we have equality for each $p \in (0, 1)$. For a proof of this, we put

$$\xi_0 = (a_0^* - b)/a, \qquad \xi_1 = (a_1^* - d)/c \tag{38}$$

and $t_0 = a^2/(a^2 + c^2)$, $t_1 = c^2/(a^2 + c^2)$. Note that $t_0 > 0$, $t_1 > 0$ and $t_0 + t_1 = 1$. Owing to the convexity of the function $f(x) = x^2$, we have

$$(t_0\xi_0 + t_1\xi_1 - p)^2 \leq t_0(\xi_0 - p)^2 + t_1(\xi_1 - p)^2. \tag{39}$$

Noticing that

$$E_p(\xi_0 - p)^2 = E_p(a_0^* - a_0)^2/a^2$$

$$E_p(\xi_1 - p)^2 = E_p(a_1^* - a_1)^2/c^2$$

and (37), we have

$$E(t_0\xi_0 + t_1\xi_1 - p)^2 \leq (a^2 + c^2)[E_p(a_0^* - a_0)^2 + E_p(a_1^* - a_1)^2] = pq/n. \tag{40}$$

But $\overline{X}_n$ is an admissible estimate for p. Hence, we must have equality in (40), and $t_0\xi_0 + t_1\xi_1 = \overline{X}_n$. Also, since x^2 is strictly convex, in order to have equality in (39), we must have $\xi_0 = \xi_1$. Therefore $\xi_0 = \xi_1 = \overline{X}_n$, and from (38) we see that $(a_0^*, a^*{}_1)$ is no other than $(a\overline{X}_n + b,\ c\overline{X}_n + d)$, and we have equality in (37) for each p. This completes the proof of Theorem 3.

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